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S E M I N A I R E

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"Integrative modeling approaches to characterize dynamics of biomolecules"

To fully understand biological functions, high-resolution biomolecular structures are required, which can be obtained through diverse experimental methods such as X-ray crystallography and, more recently, cryo-electron microscopy (cryo-EM) and computationally via AlphaFold2. While these techniques provide valuable structural insights, elucidating the dynamic of these biomolecules is also essential, given that some molecules display inherent structural flexibility through spontaneous large-domain motions. A thorough comprehension of such dynamics involves characterizing various conformational states at the atomic level. Raw experimental data from cryo-EM or high-speed atomic force microscopy (AFM) experiments consist of 2D images that represent specific views of a biomolecule, potentially capturing different conformational states, as each image may correspond to a distinct conformation. To bridge the gap between these 2D images and atomic models, simulation techniques can produce conformations in agreement with the observed data. We will introduce our efforts in developing these methods and discuss some of their applications.

Jeudi 19 décembre 2024

14h00

Salle des conférences